

3,4-Dihydroxyacetophenone
1197-09-7 | DTXSID30152546

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 118 °C

Global applicability domain: Inside

Local applicability domain index: 6.18e-01

Confidence level: 7.27e-01

Nearest Neighbors from the Training Set

Image not found

3,4-Dihydroxyacetophenone

Measured: 116

Predicted: 118

Image not found

2,4-Dihydroxybenzaldehyde

Measured: 135

Predicted: 127

Image not found

Ethanone, 1-(2,4-dihydroxyphenyl)-

Measured: 146

Predicted: 127

Image not found

Coniferyl alcohol

Measured: 74.0

Predicted: 73.8